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Building confidence in the Dirac δ -function

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Abstract

In this note we present an example from undergraduate quantum mechanics designed to highlight the versatility of the Dirac δ -function. Namely, we compute the expectation value of the Hamiltonian of a free particle in a state described by a triangular wave function $\psi(x)$. Since the first derivative of $\psi(x)$ is piecewise constant, and because this Hamiltonian is proportional to the second order spatial derivative, students often end up finding the expectation value to be zero—an unphysical answer. This problem provides a pedagogical application of the Dirac δ -function. By arriving at the same result via alternate pathways, this exercise reinforces students' confidence in the Dirac δ -function and highlights its efficiency and elegance.

Keywords: δ -function, Fourier series, Fourier transform, Hermiticity, quantum mechanics

(Some figures may appear in colour only in the online journal)

Introduction

Physics majors at most liberal arts colleges in United States generally see the Dirac δ -function during their sophomore or junior year. Its introduction is many times associated with a disclaimer that the name δ -function is a misnomer because it is not a function; it should be seen as a distribution [1, 2]. However, as all practitioners know the essential role δ -function plays in physics, it is important for the students to not only know its definition [3–6] and learn how to use it [7–9], but also to understand its subtlety [10], and verify the results of using the δ -function by alternate means, and thus incrementally build confidence in the robustness of the procedure.

Here, we present an example from undergraduate quantum mechanics [9] in which students are asked to determine the expectation value of a free-particle Hamiltonian \hat{H} in a particular state $\psi(x)$ by several methods, including one that employs the Dirac δ -function.

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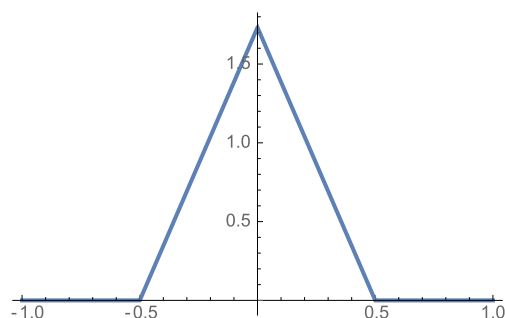


Figure 1. An isosceles triangular wave function of height $\sqrt{\frac{3}{a}}$ and extending from $-a/2$ to $+a/2$ for $a = 1$.

Description of the problem

Consider a free particle, which at $t = 0$, is in a state described by the following normalized triangular wave function

$$\psi(x) = \begin{cases} 2\sqrt{\frac{3}{a^3}}\left(x + \frac{a}{2}\right) & -\frac{a}{2} < x < 0 \\ 2\sqrt{\frac{3}{a^3}}\left(\frac{a}{2} - x\right) & 0 \leq x < \frac{a}{2} \\ 0 & |x| \geq \frac{a}{2}. \end{cases} \quad (1)$$

The isosceles triangle with its base from $-a/2$ to $+a/2$, illustrated in figure 1, is a square-integrable function, and hence is a valid wave function for any potential defined over a segment of the real-axis (or the entire real-axis) containing $[-a/2, +a/2]$.²

The Hamiltonian for the system is $\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$. Our objective is to determine the expectation value of the Hamiltonian in this state.

In our experience, when presented with this problem, many times students rush to the naive conclusion that $\langle H \rangle = -\frac{\hbar^2}{2m} \int \psi^*(x) \frac{\partial^2}{\partial x^2} \psi(x) dx = 0$, because the first derivative of the wave function is piecewise constant. They would soon realise that, because of the discontinuities of $\psi'(x)$, the second derivative of the wave function must introduce several Dirac δ -functions. This allows them to calculate the integral in a straightforward way. However, we think that students' understanding improves when alternate, equivalent solution pathways are presented. Therefore, in this paper we will use four different methods to compute the expectation value of $\langle H \rangle$. First, we consider that the free particle is inside an infinite square well of width a . Thus, $\psi(x)$ can be expressed in terms of the eigenfunctions $\phi_n(x)$ of the square well Hamiltonian. This is equivalent to the Fourier series representation of $\psi(x)$. The second method makes use of the Fourier transform of $\psi(x)$ which, up to a constant \hbar , gives the momentum space wave function $\phi(p)$. The third method uses the Hermiticity of the momentum operator [12] allowing us to cast $\langle \psi | \hat{p}^2 | \psi \rangle$ as $\langle \hat{p} \psi | \hat{p} \psi \rangle$. This turns out to be the easiest way to compute the integral. Finally, the fourth method employs the Dirac δ -function

² It is interesting to note that such a function is also the groundstate for an infinite square well potential with an attractive δ -potential in the middle [11], and for such a system its shape does not evolve with time.

mentioned above. We believe that by solving the same problem via several equivalent ways, students become more comfortable in using the Dirac δ -function and, equally important, learn to appreciate the elegance and effectiveness of such techniques.

Method 1: Fourier series

In this section we assume that the particle is free within the domain $\left(-\frac{a}{2}, \frac{a}{2}\right)$ and is blocked by infinite barriers at $x = \pm\frac{a}{2}$. The eigenfunctions are $\phi_n(x) = \sqrt{\frac{2}{a}} \cos(n\pi x/a)$ for odd n 's and $\phi_n(x) = \sqrt{\frac{2}{a}} \sin(n\pi x/a)$ for even n 's, where $n = 1, 2, 3, \dots$. As expected, they vanish at $x = \pm\frac{a}{2}$. Since the eigenfunctions $\phi_n(x)$ form a complete set, we can expand the triangular function $\psi(x)$ as the linear combination

$$\psi(x) = \sum_{n=1}^{\infty} c_n \phi_n.$$

Since $\psi(x)$ is an even function, only the cosine functions remain. Hence,

$$\psi(x) = \sum_{n=0}^{\infty} c_{2n+1} \left(\sqrt{\frac{2}{a}} \cos \left[\frac{(2n+1)\pi x}{a} \right] \right).$$

The coefficients c_{2n+1} are given by

$$\begin{aligned} c_{2n+1} &= \int_{-a/2}^{a/2} (\phi_n)^* \psi(x) dx \\ &= 2 \int_{-a/2}^0 \left(2\sqrt{\frac{3}{a^3}} \cdot \left(x + \frac{a}{2}\right) \right) \left(\sqrt{\frac{2}{a}} \cos \left[\frac{(2n+1)\pi x}{a} \right] \right) dx \\ &= \frac{4\sqrt{6}}{\pi^2(2n+1)^2}. \end{aligned}$$

The expectation value of the Hamiltonian is

$$\begin{aligned} \left\langle \frac{\hat{p}^2}{2m} \right\rangle &= -\frac{\hbar^2}{2m} \int_{-a/2}^{a/2} (\psi(x))^* \left(\frac{d^2\psi}{dx^2} \right) dx \\ &= \frac{\hbar^2}{2m} \sum_{k,n=0}^{\infty} c_{2n+1} c_{2k+1} \left(\frac{(2k+1)\pi}{a} \right)^2 \\ &\quad \times \underbrace{\int_{-a/2}^{a/2} \sqrt{\frac{2}{a}} \cos \left(\frac{(2n+1)\pi x}{a} \right) \cdot \sqrt{\frac{2}{a}} \cos \left(\frac{(2k+1)\pi x}{a} \right) dx}_{\delta_{n,k}} \\ &= \frac{\hbar^2}{2m} \sum_{n=0}^{\infty} \left(\frac{4\sqrt{6}}{\pi^2(2n+1)^2} \right)^2 \left(\frac{(2n+1)\pi}{a} \right)^2 \\ &= \frac{96\hbar^2}{2m\pi^2 a^2} \cdot \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} = \frac{96\hbar^2}{2m\pi^2 a^2} \cdot \frac{\pi^2}{8} = \frac{6\hbar^2}{ma^2}, \end{aligned} \quad (2)$$

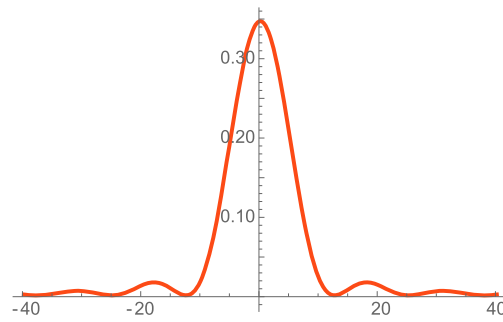


Figure 2. The momentum space wave function for $a = 1$ and $\hbar = 1$.

where we used Mathematica [13] to compute the infinite sum

$$\sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} = \frac{\pi^2}{8}.$$

Students can arrive at the same result using the formula 0.234.2 on page 7 of [14].

Method 2: Fourier transform

In this section we will use the momentum space wave function $\phi(p)$ which, up to a constant \hbar , is exactly the inverse Fourier transform of $\psi(x)$:

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x) e^{-ipx/\hbar} dx. \quad (3)$$

For the triangular wave function given in equation (1), we obtain

$$\begin{aligned} \phi(p) &= \frac{2}{\sqrt{2\pi\hbar}} \sqrt{\frac{3}{a^3}} \left(\int_{-a/2}^0 (x+a/2) e^{-ipx/\hbar} dx + \int_0^{a/2} (a/2-x) e^{-ipx/\hbar} dx \right) \\ &= \frac{1}{p^2} \sqrt{\frac{6\hbar^3}{\pi a^3}} (2 - e^{-iap/2\hbar} - e^{iap/2\hbar}) \\ &= 4 \sqrt{\frac{6\hbar^3}{\pi a^3}} \times \frac{1}{p^2} \sin^2\left(\frac{ap}{4\hbar}\right). \end{aligned} \quad (4)$$

In figure 2, we depict the momentum space wave function $\phi(p)$. In this representation, the expectation value of the Hamiltonian is

$$\left\langle \frac{\hat{p}^2}{2m} \right\rangle = \frac{1}{2m} \int_{-\infty}^{+\infty} p^2 |\phi(p)|^2 dp. \quad (5)$$

Now, inserting $\phi(p)$ from equation (4) into the above equation, we get

$$\left\langle \frac{\hat{p}^2}{2m} \right\rangle = \frac{96\hbar^3}{2m\pi a^3} \int_{-\infty}^{+\infty} \frac{1}{p^2} \sin^4\left(\frac{ap}{4\hbar}\right) dp = \frac{6\hbar^2}{ma^2}. \quad (6)$$

Again, we resorted to Mathematica [13] to calculate the integral

$$\int_{-\infty}^{+\infty} \frac{\sin^4(x)}{x^2} dx = \frac{\pi}{2}.$$

Equivalently, one can use the formula 3.821.10 from page 446 of [14].

Method 3: Hermiticity of the momentum operator

Since the momentum operator \hat{p} is Hermitian, we can write $\langle \psi | \hat{p}^2 | \psi \rangle$ as $\langle \hat{p} \psi | \hat{p} \psi \rangle$. Thus, in coordinate representation, we have

$$\begin{aligned} \left\langle \frac{\hat{p}^2}{2m} \right\rangle &= \frac{1}{2m} \langle \hat{p} \psi | \hat{p} \psi \rangle \\ &= \frac{1}{2m} \int_{-a/2}^{a/2} \left(-i\hbar \frac{d\psi}{dx} \right)^* \left(-i\hbar \frac{d\psi}{dx} \right) dx, \\ &= \frac{\hbar^2}{2m} \left(2\sqrt{\frac{3}{a^3}} \right)^2 \int_{-a/2}^{a/2} dx \\ &= \frac{6\hbar^2}{ma^2}. \end{aligned} \quad (7)$$

This method, used in [12], turns out to be the easiest of the four methods considered here.

Method 4: Dirac δ -function

Since our objective is to see an application of the δ -function, in this section we will derive the expectation value by directly applying \hat{H} to the triangular wave function of equation (1):

$$\left\langle \frac{\hat{p}^2}{2m} \right\rangle = -\frac{\hbar^2}{2m} \int_{-a/2}^{a/2} (\psi(x))^* \left(\frac{d^2\psi}{dx^2} \right) dx. \quad (8)$$

To compute this integral, we first find $\frac{d\psi}{dx}$ and $\frac{d^2\psi}{dx^2}$. The first derivative is given by

$$\frac{d\psi(x)}{dx} = \begin{cases} 2\sqrt{\frac{3}{a^3}} & -\frac{a}{2} < x < 0 \\ -2\sqrt{\frac{3}{a^3}} & 0 < x < \frac{a}{2} \\ 0 & |x| \geq \frac{a}{2}. \end{cases} \quad (9)$$

Due to the discontinuities of $\frac{d\psi}{dx}$ at $x = -a/2$, $x = 0$ and $x = a/2$, the second derivative will be a sum of three δ -functions centred on these points:

$$\frac{d^2\psi}{dx^2} = 2\sqrt{\frac{3}{a^3}} \delta\left(x + \frac{a}{2}\right) - 4\sqrt{\frac{3}{a^3}} \delta(x) + 2\sqrt{\frac{3}{a^3}} \delta\left(x - \frac{a}{2}\right). \quad (10)$$

Note that the coefficients in front of each δ -function are equal to the differences in the derivatives of ψ across each point of discontinuity.

The first and second derivatives are depicted in figure 3 for $a = 1$. Inserting equation (10) into equation (8), and taking into account that $\psi\left(\pm\frac{a}{2}\right) = 0$, we get

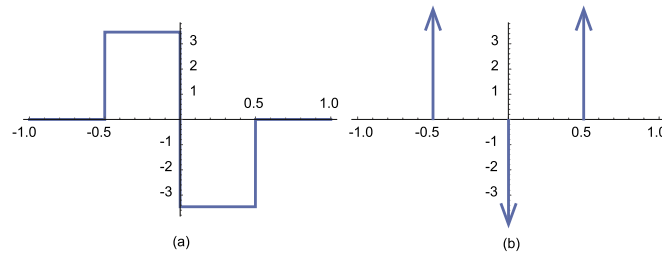


Figure 3. The first derivative (a) and second derivative (b) of $\psi(x)$ for $a = 1$. The δ -functions are represented by vertical arrows.

$$\begin{aligned}
 \left\langle \frac{\hat{p}^2}{2m} \right\rangle &= -\frac{\hbar^2}{2m} \int_{-a/2}^{a/2} \psi^*(x) \left[2\sqrt{\frac{3}{a^3}} \delta\left(x + \frac{a}{2}\right) - 4\sqrt{\frac{3}{a^3}} \delta(x) + 2\sqrt{\frac{3}{a^3}} \delta\left(x - \frac{a}{2}\right) \right] dx \\
 &= -\frac{\hbar^2}{2m} \left[\psi^*\left(-\frac{a}{2}\right) \left(2\sqrt{\frac{3}{a^3}} \right) - (\psi(0))^* \left(-4\sqrt{\frac{3}{a^3}} \right) - \psi^*\left(\frac{a}{2}\right) \left(2\sqrt{\frac{3}{a^3}} \right) \right] \\
 &= -\frac{\hbar^2}{2m} \cdot \left(2\sqrt{\frac{3}{a^3}} \cdot \frac{a}{2} \right) \left(-4\sqrt{\frac{3}{a^3}} \right) \\
 &= \frac{6\hbar^2}{ma^2}.
 \end{aligned} \tag{11}$$

Note that this derivation is also straightforward and, unlike the first two methods, does not require any use of Mathematica.

Conclusion

In this note we computed the expectation value of a free-particle Hamiltonian in a state described by a triangular wave function $\psi(x)$. Since the first derivative of $\psi(x)$ is piecewise constant, and because the Hamiltonian is proportional to a second order spatial derivative, students often end up finding the expectation value to be zero—an unphysical answer. This problem provides a natural setting for the introduction of Dirac δ -function as the derivative of a step function. By computing the expectation value of the Hamiltonian via several different methods we attempt to bolster their confidence in δ -function, which appears in many areas of physics.

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